

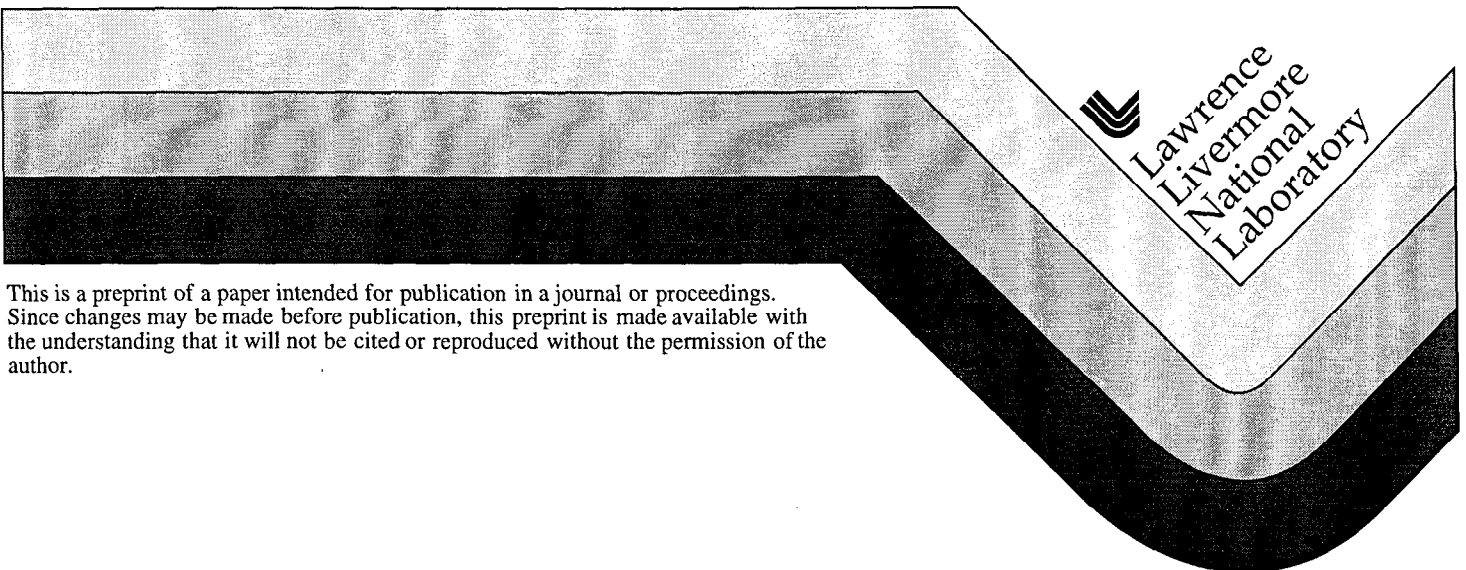
UCRL-JC-133660  
PREPRINT

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This paper was prepared for submittal to the  
International Conference on Mathematics and Computation,  
Reactor Physics, and Environmental Analysis in Nuclear Applications  
Madrid, Spain  
September 27-30, 1999

**March 1999**



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# The Excess Mean Free Path Transport Condensed History Algorithm

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## Abstract

A new Condensed History algorithm is introduced to enhance the Monte Carlo simulation of electron transport problems. Unlike established multiple scattering algorithms, this method is a true transport process – it simulates a transport equation that approximates the exact Boltzmann equation. The new equation has a larger mean free path than, and preserves two angular moments of, the Boltzmann equation. Thus, the new equation conserves both particles and scattering power, and it is more efficient to model by Monte Carlo. We show that this “Transport Condensed History” algorithm more accurately predicts electron position as a function of path length traveled (energy lost) than current Condensed History schemes. We also show that it can move particles across material boundaries and interfaces with acceptable accuracy and efficiency.

## 1 Introduction

Most analog simulations of electron transport problems require exhaustive amounts of time to provide reasonable results. This is because electrons can undergo up to  $10^5$  collisions during their lifetime, and analog methods must simulate each of these collisions faithfully according to the true physics.

Condensed History algorithms are approximate Monte Carlo methods designed to remedy this problem. They make use of the fact that most collisions between electrons and atoms occur very close together and result in very small changes in direction and energy loss. Instead of modeling every interaction, Condensed History algorithms account for the cumulative effect of multiple collisions in a single “step” of (user-specified) path length  $s$ . Because computational cost is proportional to the total number of steps, the largest step size possible within the constraint of acceptable accuracy is desired.

The first multiple scattering algorithms were developed by Martin Berger (Berger, 1963). In this paper, Berger devised two methods that are based on the strategy of artificially decoupling

the streaming, angular scattering, and energy loss processes of the transport equation. In each Condensed History (CH) step, these processes are executed separately. The CH streaming process determines the Monte Carlo electron's new position, the CH angular scattering process finds the new direction of flight, and the CH energy loss or slowing down process determines the new energy. Berger's first method implements the processes in the order stated over the entire step  $s$ . Recognizing that this forces the electron's new position to lie along the original direction of flight such that no transverse displacement occurs, Berger formulated a second algorithm. There, the streaming process is split into two sub-steps, each with length  $s/2$ . Larsen has shown that if the slowing down process is also split into sub-steps, Berger's second method has a higher order of accuracy than his first (Larsen, 1992). Recently, Baro et al. have developed the PENELOPE algorithm, which is identical to Berger's second method except that the first sub-step has length  $\xi s$  while the second has length  $(1 - \xi)s$ , where  $\xi$  is a uniformly distributed random number from  $0 < \xi < 1$  (Baro, 1995).

Comparisons with physical experiments have shown that these traditional CH algorithms yield accurate results for many problems. Nevertheless, for some situations, the weaknesses of these methods appear. One such situation occurs when electrons have slowed down to energies in the keV range, especially in high atomic number materials. Here, the angular scattering is only moderately anisotropic. Generally, when the electron's initial and final directions in a step are not nearly identical, the CH streaming process does not accurately determine the electron's position.

Another weakness of established CH methods is that their theoretical basis requires an infinite, homogeneous medium. These methods have difficulty simulating practical problems that contain complicated geometries and/or many material regions. Substantial errors often arise when trying to move particles across the boundaries or interfaces between regions. Bielajew has created the PRESTA algorithm to handle this difficulty (Bielajew, 1996). This algorithm automatically shrinks the step size as the electron history approaches a boundary. When the particle actually reaches a boundary, the step size has been reduced to the point where single scatter Monte Carlo is used to move it across. PRESTA provides accurate results, but it is often time-consuming. Thus, simulations can be quite inefficient for problems involving many interfaces.

In this paper, we describe a new CH algorithm that copes with these difficulties. Unlike conventional Condensed History, the new method is a direct Monte Carlo simulation of a transport process. This process is described by a transport equation that approximates the true Boltzmann equation with a larger mean free path and a more isotropic scattering operator. Previously, we have developed an algorithm in which the user specifies the mean free path, but this method does not limit to the true Boltzmann solution as this path length shrinks to  $1/\Sigma_t$  (Tolar, 1999). The mean free path, however, of our new "Transport Condensed History" (TCH) scheme is

$$\lambda_{TCH} = \frac{1}{\Sigma_t} + s ,$$

where  $s$  is a parameter representing the "excess mean free path". The user is free to specify this parameter; as  $s \rightarrow 0$ , the exact Boltzmann transport process is recovered. In addition, the zero-th and first order angular moments of the modified scattering operator are identical to the true scattering operator. For an infinite medium, H.W. Lewis has shown that if the  $n$ -th order

angular moments of two scattering kernels agree, then the  $n$ -th order space-angle moments of the solutions of the two transport equations that contain these kernels will also agree (Lewis, 1950). Therefore, TCH predicts the mean position of particles that have traveled a given path length exactly, regardless of their energy or how anisotropically they scatter.

Because it is a transport process, the TCH algorithm is implemented just like an analog Monte Carlo; no additional logic or special treatment is necessary to move particles across boundaries and interfaces. The TCH method can model heterogeneous, finite medium problems effectively and efficiently because of its large mean free path. In the next section we derive the TCH scheme, describe its features, and explain how it is implemented in a Monte Carlo code. Then, we present numerical results from several test problems to validate our analysis. We conclude with a brief discussion.

## 2 Transport Condensed History Theory

To simplify the analysis, we consider the one-group transport equation with no absorption ( $\Sigma_t = \Sigma_{s0}$ ):

$$\underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega}) + \Sigma_{s0} \psi(\underline{r}, \underline{\Omega}) + \int_{4\pi} \Sigma_s (\underline{\Omega} \cdot \underline{\Omega}') \psi(\underline{r}, \underline{\Omega}') d\Omega' = 0. \quad (1)$$

Performing Legendre polynomial  $P_n(\underline{\Omega} \cdot \underline{\Omega}')$  expansions for the angular flux and the differential scattering cross section, we obtain

$$\psi(\underline{r}, \underline{\Omega}) = \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) \int_{4\pi} P_n(\underline{\Omega} \cdot \underline{\Omega}') \psi(\underline{r}, \underline{\Omega}') d\Omega', \quad (2)$$

and

$$\Sigma_s(\mu_0) = \Sigma_{s0} \left[ \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) c_n P_n(\mu_0) \right], \quad (3)$$

where

$$c_n = \frac{\Sigma_{sn}}{\Sigma_{s0}}, \quad (4)$$

and

$$\mu_0 = \underline{\Omega} \cdot \underline{\Omega}'. \quad (5)$$

Thus, we can write Eq. 1 as

$$\underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega}) + \Sigma_{s0} \mathcal{L} \psi(\underline{r}, \underline{\Omega}) = 0. \quad (6)$$

In this equation,  $\Sigma_{s0} \mathcal{L}$  is the outscattering-minus-inscattering operator:

$$\Sigma_{s0} \mathcal{L} \psi(\underline{r}, \underline{\Omega}) \equiv \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) \left( \frac{1-c_n}{\lambda} \right) \int_{4\pi} P_n(\underline{\Omega} \cdot \underline{\Omega}') \psi(\underline{r}, \underline{\Omega}') d\Omega', \quad (7)$$

where

$$\lambda \equiv \frac{1}{\Sigma_{s0}} = \text{mean free path} . \quad (8)$$

### 2.1 The Excess Mean Free Path

Let  $s$  be a positive constant called the “excess mean free path,” and let the constants  $a_n(s)$  satisfy

$$\frac{1 - c_n}{\lambda} = \frac{1 - a_n(s)}{\lambda + s} , \quad n \geq 0 . \quad (9)$$

Solving for  $a_n(s)$ , we obtain

$$a_n(s) = 1 - (1 - c_n) \left(1 + \frac{s}{\lambda}\right) . \quad (10)$$

Using Eqs. 7 and 9, we can write

$$\begin{aligned} \Sigma_{s0} \mathcal{L} \psi(r, \underline{\Omega}) &\equiv \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) \left( \frac{1 - a_n(s)}{\lambda + s} \right) \int_{4\pi} P_n(\underline{\Omega} \cdot \underline{\Omega}') \psi(r, \underline{\Omega}') d\Omega' \\ &= \frac{1}{\lambda + s} \left[ \psi(r, \underline{\Omega}) - \int_{4\pi} f_s(\underline{\Omega} \cdot \underline{\Omega}') \psi(r, \underline{\Omega}') d\Omega' \right] , \end{aligned} \quad (11)$$

where

$$f_s(\mu_0) \equiv \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) a_n(s) P_n(\mu_0) . \quad (12)$$

Eqs. 11 and 6 now give

$$\underline{\Omega} \cdot \underline{\nabla} \psi(r, \underline{\Omega}) + \frac{1}{\lambda + s} \psi(r, \underline{\Omega}) = \frac{1}{\lambda + s} \int_{4\pi} f_s(\underline{\Omega} \cdot \underline{\Omega}') \psi(r, \underline{\Omega}') d\Omega' . \quad (13)$$

Eq. 13 is algebraically equivalent to the original transport equation defined in Eq. 1. The formal mean free path of Eq. 13 is  $(\lambda + s)$ , which is greater than the original mean free path by an amount  $s$ . Unfortunately, the function  $f_s(\mu_0)$  is not positive, and it contains a delta function. As it stands, Eq. 13 does not describe a transport process with mean free path  $(\lambda + s)$ .

### 2.2 The Transport Condensed History Approximation

The essence of the Transport Condensed History approximation is to replace the non-positive singular function  $f_s(\mu_0)$  by a “nicer” function

$$F_s(\mu_0) = \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) b_n(s) P_n(\mu_0) , \quad (14)$$

which has the following properties:

1.  $F_s(\mu_0)$  is a bounded, positive function of  $\mu_0$ . Then Eq. 13, with  $f_s(\mu_0)$  replaced with  $F_s(\mu_0)$ , will be a true transport process.

2.  $\lim_{s \rightarrow 0} b_n(s) = c_n$ . Thus, the approximate transport process reduces to the Boltzmann process as the excess mean free path shrinks to zero.
3.  $|b_n(s) - a_n(s)| = \mathcal{O}(s^N)$ , where  $N$  is large. This will help minimize the error.
4.  $b_n(s) = a_n(s)$  ,  $0 \leq n \leq M$ , where  $M$  is large. This condition will preserve  $M + 1$  angular moments of the original scattering process.

We have devised a scheme in which  $N = 1$  and  $M = 1$ . To begin, we rewrite Eq. 10 as

$$a_n(s) = c_n \left[ 1 - \left( \frac{1 - c_n}{c_n} \right) \frac{s}{\lambda} \right] . \quad (15)$$

Now, we define the functions  $b_n(s)$  by:

$$b_n(s) \equiv c_n \exp \left[ -(1 - c_n) \frac{s_1}{\lambda} \right] , \quad (16)$$

where  $s_1$  is defined in terms of  $s$  by

$$1 - \left( \frac{1 - c_1}{c_1} \right) \frac{s}{\lambda} = \exp \left[ -(1 - c_1) \frac{s_1}{\lambda} \right] . \quad (17)$$

Recognizing that  $c_1 = \bar{\mu}$  = mean scattering cosine for the exact transport process, we can solve Eq. 17 for  $s$  in terms of  $s_1$ :

$$\begin{aligned} s &= \frac{\lambda \bar{\mu}}{1 - \bar{\mu}} \left\{ 1 - \exp \left[ -(1 - \bar{\mu}) \frac{s_1}{\lambda} \right] \right\} \\ &= (\lambda_{tr} - \lambda) \left[ 1 - \exp \left( -\frac{s_1}{\lambda_{tr}} \right) \right] . \end{aligned} \quad (18)$$

Here  $\lambda_{tr}$  is the transport mean free path of the original transport equation:

$$\lambda_{tr} = \frac{\lambda}{1 - \bar{\mu}} = \frac{1}{\Sigma_{s0} (1 - \bar{\mu})} . \quad (19)$$

Eq. 18 imposes the following constraint:

$$\lambda + s < \lambda_{tr} . \quad (20)$$

Physically,  $\lambda_{tr}$  is the mean penetration depth of particles that have traveled infinite path length. Therefore, Eq. 20 only requires that the mean free path of the TCH scheme be less than this maximum mean distance of flight. This constraint does not forbid reasonable choices for  $s$ . In practice, we choose  $s_1$  to be any suitable positive length, and then use Eq. 18 to determine the excess mean free path  $s$ .

Eqs. 15-17 reveal that

$$b_n(s) = a_n(s) \quad n = 0, 1 .$$

Also, for  $s \approx 0$ , we can solve Eq. 17 to see that  $s_1 \approx s/\bar{\mu} = \mathcal{O}(s)$ . From Eq. 16,

$$b_n(s) = c_n [1 + \mathcal{O}(s)] .$$

Hence,  $|b_n(s) - a_n(s)| = \mathcal{O}(s)$ , and  $\lim_{s \rightarrow 0} b_n(s) = c_n$ , as desired.

Figure 1 compares the constants  $a_n(s)$  and  $b_n(s)$  for 50 keV electrons in aluminum. The path length  $s_1$  is about 25 mean free paths and corresponds to an energy loss of 1.25 keV. As indicated,  $a_n(s)$  and  $b_n(s)$  agree for  $n = 0$  and  $n = 1$ , and they remain close together for small  $n$ . Then, they begin to depart from one another; for large  $n$ ,  $b_n(s) \rightarrow 0$  and  $a_n(s) \rightarrow -s/\lambda \approx -25$ .

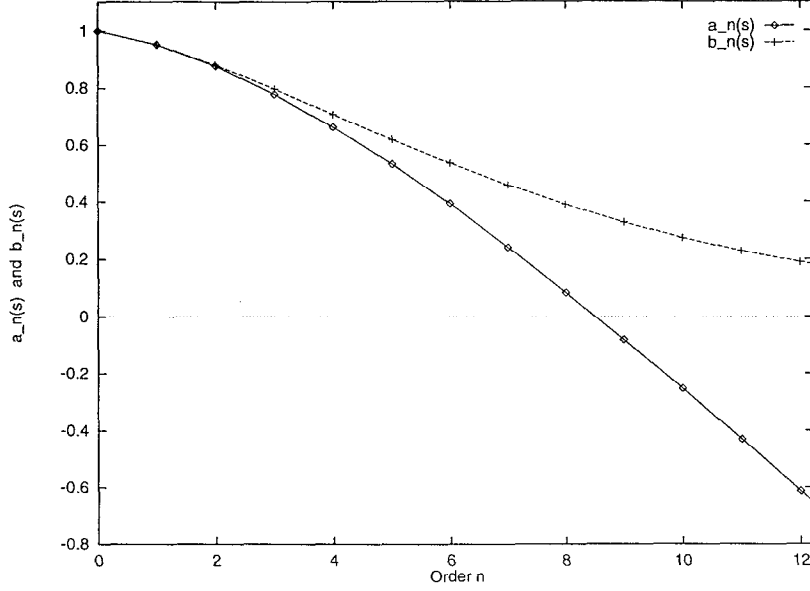


Figure 1:  $a_n(s)$  and  $b_n(s)$  Vs.  $n$  for 50 keV Electrons in Aluminum

### 2.3 The New Scattering Kernel

The remaining task is to examine the positivity of the scattering kernel  $F_s(\mu_o)$  in the TCH equation. Using Eq. 14 and 16, this function is given by

$$F_s(\mu_o) = \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) c_n \exp \left[ -(1 - c_n) \frac{s_1}{\lambda} \right] P_n(\mu_o) . \quad (21)$$

We observe that  $F_s(\mu_o)$  is the convolution of two different scattering kernels. The first,

$$g(\mu_o) = \frac{1}{\Sigma_{s0}} \Sigma_s(\mu_o) = \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) c_n P_n(\mu_o) , \quad (22)$$

describes single-collision scattering. Physically,  $g(\mu_o)$  is the probability distribution function for an electron's direction of flight after undergoing one scattering event. This function appears in the Boltzmann equation and is positive for  $-1 \leq \mu_o \leq 1$ . The second function,

$$G_s(\mu_o) = \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) \exp \left[ -(1 - c_n) \frac{s_1}{\lambda} \right] P_n(\mu_o) , \quad (23)$$

describes multiple scattering. Physically, it is the probability distribution function for an electron's direction of flight after traveling a path length  $s_1$ . This function is called the Goudsmit-Saunderson distribution (Goudsmit, 1940), and is positive. Since  $F_s(\mu_o)$  is the convolution



$$F_s(\underline{\Omega} \cdot \underline{\Omega}') = \int_{4\pi} g(\underline{\Omega} \cdot \underline{\Omega}'') G_s(\underline{\Omega}'' \cdot \underline{\Omega}) d\Omega'' \quad (24)$$

of the two positive functions  $g$  and  $G_s$ , it must itself be positive.

## 2.4 Implementation

The Transport Condensed History algorithm is simulated just like a standard analog Monte Carlo code. To begin, the user specifies the path length  $s_1$ , and the excess mean free path  $s$  is calculated from Eq. 18. Next, the distance to “collision” (in mean free paths) is sampled from an exponential distribution with mean value  $1 + s/\lambda$ . The particle travels this entire distance in its initial direction whether it crosses a boundary or not. After the electron has reached its new position, the new direction of flight is sampled from  $F_s(\mu_0)$ . This is done by sampling a direction from  $g(\mu_0)$  given by Eq. 22 and then, without moving the particle, sampling another direction  $G_s(\mu_0)$  given by Eq. 23. Thus, the new direction of flight is the cumulative effect from a single and a multiple scattering event. Lastly, the electron’s energy after the collision is determined by the Continuous Slowing Down approximation. That is, energy loss is directly proportional to path length traveled and is obtained using the electron’s stopping power. This process is repeated until the electron history is terminated.

## 3 Numerical Results

### 3.1 Aluminum Problem

To test the Transport Condensed History (TCH) algorithm, we consider a pencil beam of 150 keV electrons initially traveling in the  $z$ -direction in an infinite medium of aluminum. The Continuous Slowing Down approximation is employed with multigroup cross sections and stopping powers obtained from the EPICSHOW code (Cullen, 1997). We do not consider discrete energy loss events or any secondary particle production. Elastic scattering events are modeled by the Screened Rutherford kernel (Bielajew, 1998). As the electrons slow down to various energies, we calculate the mean position and the standard deviation about this mean. Three methods are used to obtain these quantities: (1) TCH, (2) PENELOPE (PEN), and (3) analog Monte Carlo.

For TCH and PEN,  $s_1$  is selected as 1/4 the path length required for an electron to lose the energy of one group. Each history is terminated after traveling through 35 groups to 1.0 keV. Analog Monte Carlo electrons typically undergo about 2800 collisions per history, while TCH and PEN particles undergo about 140 steps per history (4 per energy group). Thus, each step is on the average 20 mean free paths.

The results are shown in Figure 2. We see excellent agreement between both Condensed History methods and analog Monte Carlo. For TCH, this is expected because the algorithm preserves two angular moments of the Boltzmann scattering operator. Thus, TCH determines the mean depth,  $\langle z \rangle$ , exactly for any infinite medium problem. Although TCH does not preserve second order moments, TCH calculates the standard deviation about the mean depth,  $\text{sig}_z = \sigma_z$ , the mean radius,  $\langle r \rangle = \langle \sqrt{x^2 + y^2} \rangle$ , and the root mean squared radius,  $\text{rms} = \sigma_r = \sqrt{\sigma_x^2 + \sigma_y^2}$ , within 2% of the analog values. The PEN results are also within 2% of the analog values because the electrons in this energy range scatter fairly anisotropically in aluminum. (The mean cosines for single scattering events are approximately  $\bar{\mu} = 0.998$ .)

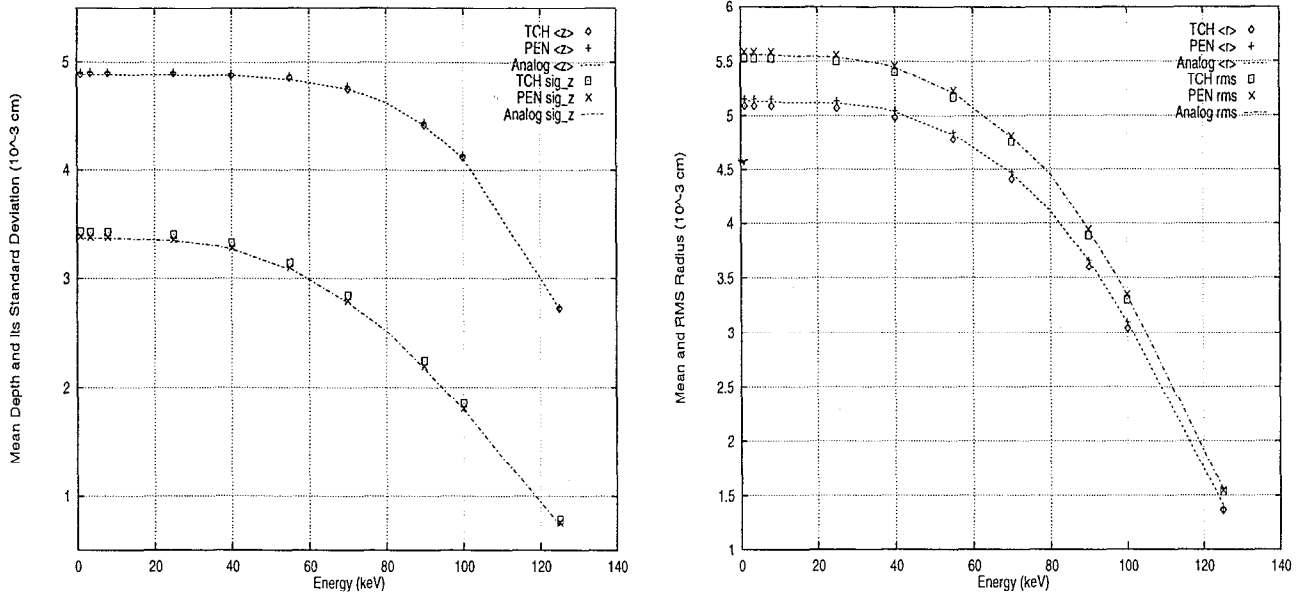


Figure 2: (a) Mean Depth and Its Standard Deviation and (b) Mean and RMS Radius Vs. Energy for a 150 keV Electron Beam in Aluminum

### 3.2 Gold Problem

Next we consider the same problem, except that the electrons travel in an infinite medium of gold. Here, the average step size is about 32 mean free paths for TCH and PEN. Because gold has a much higher atomic number than aluminum, the electrons scatter more isotropically; the mean cosines for single scattering are roughly  $\bar{\mu} = 0.987$ . Table 1 compares  $\langle z \rangle$ ,  $\sigma_z$ , and  $\sigma_r$  for a few energies. For  $\langle z \rangle$ , we see excellent agreement between analog Monte Carlo and TCH, but now the PEN results are off by about 8%. Also, the TCH estimates for  $\sigma_z$  and  $\sigma_r$  are slightly closer than PEN to the analog values.

### 3.3 Aluminum - Gold Interface Problem

The last problem contains a planar interface at the depth  $z = 4.0 \times 10^{-4}$  cm. To the left of the interface, the electrons slow down in gold, and on the right, in aluminum. The 150 keV electron beam starts at  $z = 0$ , traveling monodirectionally down the  $z$ -axis. For CH methods, the average step is around 29 mean free paths. For the PEN scheme, we do not implement the PRESTA algorithm to shrink or expand the step sizes near the interface. Although the procedure of moving electrons  $\xi s/\lambda$  and  $(1 - \xi)s/\lambda$  mean free paths between collisions is not rigorously correct across the interface, Bielajew suggests that it should be fairly accurate.

Figure 3 clearly indicates the superiority of TCH for this problem. Generally, the TCH measurements are within 3% while the PEN results are only within about 10% of the analog results. Since this problem contains two regions of different materials, TCH cannot predict  $\langle z \rangle$  exactly; moments can only be preserved in an infinite medium. Nevertheless, the errors in TCH associated with moving electrons across the interface are apparently less than those errors in PEN. To

Table 1: Mean Depth and Standard Deviations for a 150 keV Electron Beam in Gold

Final Energy (keV)	Solution Method	$\langle z \rangle$ ( $10^{-3}\text{cm}$ )	$\sigma_z$ ( $10^{-3}\text{cm}$ )	$\sigma_r$ ( $10^{-3}\text{cm}$ )
125.0	Analog	0.1960	0.2402	0.3640
125.0	TCH	0.1962	0.2550	0.3538
125.0	PEN	0.2106	0.2584	0.3788
70.0	Analog	0.1995	0.4356	0.6306
70.0	TCH	0.1997	0.4445	0.6243
70.0	PEN	0.2146	0.4618	0.6620
40.0	Analog	0.1995	0.4587	0.6625
40.0	TCH	0.1997	0.4670	0.6565
40.0	PEN	0.2146	0.4847	0.6941
1.0	Analog	0.1995	0.4634	0.6690
1.0	TCH	0.1998	0.4715	0.6632
1.0	PEN	0.2146	0.4895	0.7006

achieve greater accuracy for either scheme, the step sizes must be reduced. For the simulations we have described, TCH and PEN are equally efficient; both are about ten times faster than analog Monte Carlo.

#### 4 Conclusions

In summary, we have developed a new Condensed History algorithm for electrons that is a transport process. The mean free path of this process is the sum of the mean free path given by the Boltzmann equation plus the excess mean free path  $s$  specified by the user. If  $s = 0$ , the TCH transport process reduces to the physical transport process. The TCH algorithm has been tested for pencil beams with continuous slowing down energy dependence. We have shown that the TCH algorithm predicts the locations of electrons of a given energy accurately. Also, we have shown that TCH is adequate for a problem involving a material interface without including the costly expense of shrinking the step sizes.

Overall, the TCH method is designed to improve the accuracy/efficiency of current Condensed History methods. The TCH method may provide substantial contributions to electron transport problems in medical physics, especially for high accuracy applications such as radiotherapy and radiation dosimetry. In the future, we plan to test the TCH method under more practical situations that include complicated geometries with many material regions. We also hope to develop more advanced TCH models that have a higher order of accuracy and preserve additional angular moments of the Boltzmann equation.

#### Acknowledgments

This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract W-7405-ENG-48.

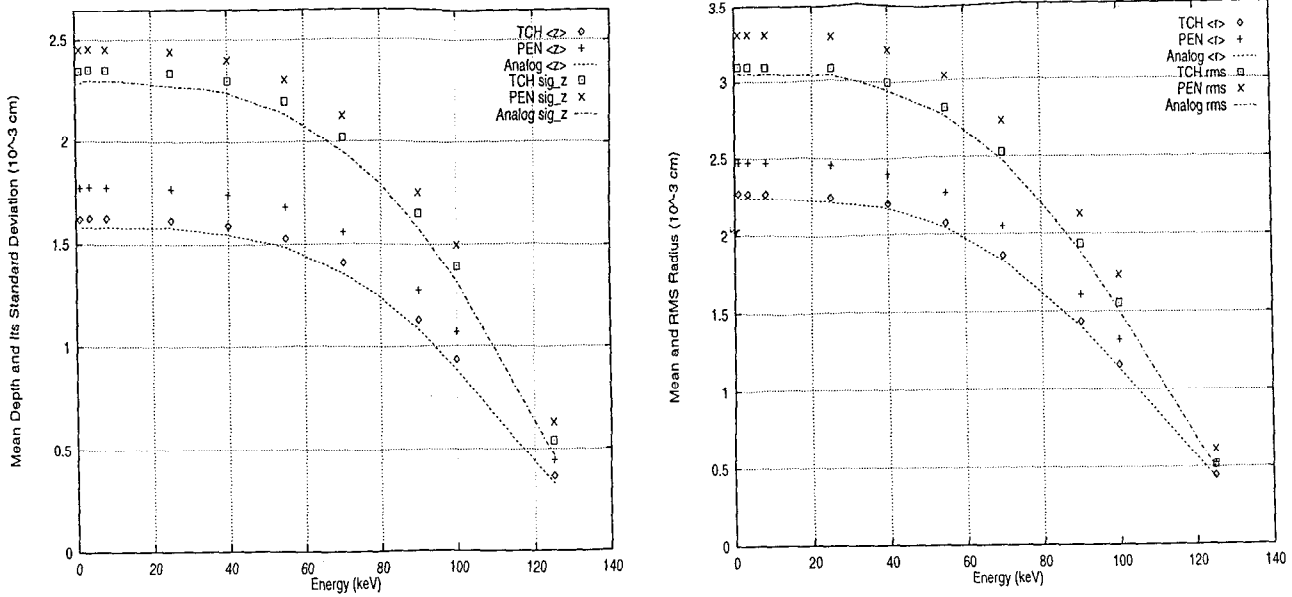


Figure 3: (a) Mean Depth and Its Standard Deviation and (b) Mean and RMS Radius Vs. Energy for a 150 keV Electron Beam in Gold and Aluminum

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